**Supporting information for**

Structures, energetics, and IR spectra of monohydrated inorganic acids: *Ab initio* and *DFT study*

Maciej Kołaski, Aleksey A. Zakharenko, S. Karthikeyan, and Kwang S. Kim

**Contents:**

Table S1
Table S2
Table S3
Table S4
Table S5

**Table S1.** MP2(B3LYP)/aVDZ zero-point energy (ZPE) corrected binding energies ($-\Delta E_0$), binding enthalpies ($-\Delta H_r$) and free binding energies ($-\Delta G_r$) [in kJ/mol] at room temperature and 1 bar for various conformers of inorganic acid···water complexes.

| acid···water | conformer | $-\Delta E_0$ | $-\Delta H_r$ | $-\Delta G_r$ |
|---|---|---|---|---|
| **$HBO_2$···$H_2O$** | **A** | **33.9(32.3)** | **35.7(34.1)** | **6.0(4.5)** |
| **$H_3BO_3$···$H_2O$** | **$AD_{OH}$** | **28.2(22.0)** | **30.4(24.1)** | **-6.7(-12.9)** |
| **HCN···$H_2O$** | **$A_H$** | **18.8(16.6)** | **18.7(16.7)** | **-5.0(-8.3)** |
| | $D_N$ | 12.6(9.4) | 13.4(10.2) | -11.1(-14.4) |
| **$HNO_2$···$H_2O$** | **$A(D_O)$** | **23.6(21.1)** | **25.2(22.7)** | **-8.7(-11.1)** |
| | A | 22.3(20.2) | 23.0(20.7) | -6.5(-8.6) |
| | $D_{OH}$ | 10.7(-) | 10.5(-) | -14.6(-) |
| | $D_O$ | 5.1(2.3) | 4.1(1.6) | -17.4(-20.6) |
| **$HNO_3$···$H_2O$** | **$AD_O$** | **34.1(31.4)** | **35.9(33.5)** | **0.0(-2.5)** |
| | $D_{OH}W_{NO}$ | 12.4(-) | 11.0(-) | 13.2(-) |
| | $D_O{}^2$ | 7.5(3.4) | 6.4(2.4) | -12.8(-20.6) |
| | $D_O$ | 6.7(3.3) | 5.8(2.2) | -17.2(-20.5) |
| **$P(OH)_3$···$H_2O$** | **$AD_{OH}W_{PO}$** | **30.4(21.3)** | **33.3(24.2)** | **-6.0(-15.1)** |
| | A | 11.5(7.3) | 11.3(7.0) | -14.0(-18.2) |
| **$H_3PO_3$···$H_2O$** | **$AD_OW_{PO}$** | **45.4(37.5)** | **47.4(41.4)** | **6.6(0.1)** |
| | $AD_{OH}W_{PO}$ | 25.4(19.1) | 28.0(21.5) | -10.2(-15.1) |
| | $D_{OH}{}^2W_{PO}$ | 13.4(5.6) | 13.6(5.1) | -19.0(-22.5) |
| | $D_{OH}W_{PO}$ | 12.7(6.6) | 12.7(6.3) | -16.4(-21.0) |
| **$H_3PO_4$···$H_2O$** | **$AD_OW_{PO}$** | **44.0(37.5)** | **47.5(41.2)** | **8.1(1.0)** |
| | $AD_{OH}W_{PO}$ | 30.3(23.0) | 32.9(25.5) | -5.2(-12.0) |
| **$H_2S$···$H_2O$** | **$D_S$** | **8.0(4.4)** | **8.5(5.1)** | **-14.9(-17.7)** |
| | $A_H$ | 8.0(4.4) | 7.7(4.0) | -14.3(-15.9) |
| **$(HO)_2SO$···$H_2O$** | **$A^2D_OW_{SO}$** | **37.4(28.1)** | **41.2(31.6)** | **-0.7(-8.2)** |
| | $AD_OW_{SO}$ | 34.6(27.5) | 38.0(31.0) | -2.4(-9.4) |
| | $AD_{OH}W_{SO}$ | 27.9(19.5) | 30.2(21.5) | -7.8(-16.2) |
| | $D_{OH}{}^2W_{SO}$ | 12.2(3.9) | 12.3(3.3) | -19.4(-23.3) |
| | $D_{OH}W_{SO}$ | 10.3(5.2) | 9.9(4.5) | -16.0(-18.8) |
| **$H_2SO_3$···$H_2O$** | **$AD_OW_{SO}$** | **42.1(36.4)** | **45.2(39.6)** | **6.5(0.8)** |
| | $AD_O{}^2W_{SO}$ | 22.7(-) | 22.5(-) | -5.7(-) |
| | $A_H$ | 21.2(17.8) | 19.8(16.6) | -3.3(-8.5) |
| **$H_2SO_4$···$H_2O$** | **$AD_OW_{SO}$** | **43.5(37.0)** | **46.3(38.8)** | **7.8(1.6)** |
| | $A^2D_OW_{SO}$ | 37.1(26.8) | 40.1(29.6) | 0.3(-7.8) |
| | $D_O$ | 7.2(2.9) | 5.9(1.0) | -16.4(-15.7) |
| **$H_2Se$···$H_2O$** | **$D_{Se}$** | **8.8(3.4)** | **9.1(4.1)** | **-14.2(-19.2)** |
| | $A_H$ | 7.1(3.0) | 6.4(2.0) | -14.6(-15.6) |

**Table S2.** MP2(B3LYP)/aVDZ zero-point energy (ZPE) corrected binding energies ($-\Delta E_0$), binding enthalpies ($-\Delta H_r$) and free binding energies ($-\Delta G_r$) [in kJ/mol] at room temperature and 1 bar for various conformers of monohydrated inorganic acids containing halogen atoms.

| acid···water | conformer | $-\Delta E_0$ | $-\Delta H_r$ | $-\Delta G_r$ |
|---|---|---|---|---|
| **HF···$H_2O$** | **$A_H$** | **26.3(26.8)** | **30.8(31.1)** | **1.0(1.6)** |
| **HCl···$H_2O$** | **$A_H$** | **17.5(14.6)** | **20.7(18.0)** | **-7.4(-10.6)** |
| **HClO···$H_2O$** | **A** | **24.8(21.6)** | **26.3(23.1)** | **-1.8(-5.7)** |
| | $E_{ClO}$ | 8.8(5.3) | 8.2(4.7) | -19.0(-22.3) |
| **$HClO_2$···$H_2O$** | **$AD_OE_{ClO}$** | **35.5(31.2)** | **38.7(34.4)** | **-0.7(-4.9)** |
| | $D_OW_{ClO}$ | 15.2(11.5) | 15.9(11.8) | -13.9(-15.6) |
| | $D_{OH}E_{ClO}$ | 15.8(6.7) | 16.0(6.2) | -15.2(-22.0) |
| **$HClO_3$···$H_2O$** | **$AD_OW_{ClO}$** | **30.0(29.1)** | **33.3(32.4)** | **-6.1(-6.7)** |
| | $D_{OH}E_{ClO}$ | 21.2(8.7) | 22.0(8.3) | -11.4(-21.5) |
| | $D_O{}^2E_{ClO}$ | 18.4(10.7) | 17.5(9.8) | -9.4(-17.1) |
| | $D_{OH}$ | 12.5(-) | 12.5(-) | -14.1(-) |
| **$HClO_4$···$H_2O$** | **$AD_O{}^2W_{ClO}$** | **39.4(35.6)** | **41.9(37.7)** | **4.9(3.6)** |
| | $AD_OW_{ClO}$ | 37.7(34.1) | 40.0(36.3) | 3.4(0.0) |
| | $D_O$ | 6.5(1.6) | 4.9(-0.1) | -15.0(-21.0) |
| **HBr···$H_2O$** | **$A_H$** | **15.3(11.5)** | **17.9(14.3)** | **-9.2(-13.3)** |
| | $W_{BrO}$ | 3.9(0.5) | 3.9(-0.3) | -15.7(-14.0) |
| **HBrO···$H_2O$** | **A** | **24.1(19.7)** | **25.4(21.0)** | **-0.4(-7.6)** |
| | $E_{BrO}$ | 16.1(10.9) | 15.8(10.9) | -13.4(-18.9) |
| | $D_{OH}$ | 11.5(-) | 12.0(-) | -13.5(-) |
| **$HBrO_2$···$H_2O$** | **$AD_OW_{BrO}$** | **38.5(32.8)** | **41.5(34.4)** | **2.1(-5.0)** |
| | $D_OE_{BrO}$ | 22.6(14.7) | 23.0(15.2) | -9.5(-17.7) |
| | $D_OW_{BrO}$ | 19.8(14.2) | 20.8(14.6) | -10.3(-11.8) |
| | $D_{OH}E_{BrO}$ | 20.9(10.2) | 21.3(10.0) | -11.8(-20.4) |
| **$HBrO_3$···$H_2O$** | **$AD_OW_{BrO}$** | **37.1(32.6)** | **40.6(36.2)** | **1.0(-4.0)** |
| | $D_O{}^2E_{BrO}$ | 27.2(18.2) | 27.5(18.6) | -5.2(-14.2) |
| | $D_OD_{OH}E_{BrO}$ | 26.2(14.8) | 27.2(15.3) | -8.3(-17.8) |
| **$HBrO_4$···$H_2O$** | **$AD_OW_{BrO}$** | **44.0(37.2)** | **47.1(40.5)** | **7.8(0.2)** |
| | $AD_OW_{BrO}$ | 42.6(36.8) | 45.5(40.1) | 7.1(0.3) |
| **HI···$H_2O$** | **$A_H$** | **11.6(6.3)** | **12.9(7.8)** | **-10.7(-16.5)** |
| | $D_I$ | 11.1(3.5) | 12.2(3.5) | -10.1(-15.1) |
| | $W_{IO}$ | 7.6(4.2) | 7.6(5.1) | -12.5(-18.7) |
| **HIO···$H_2O$** | **$E_{IO}$** | **24.7(22.0)** | **24.7(22.5)** | **-6.1(-9.3)** |
| | A | 21.8(16.7) | 22.8(17.9) | -4.3(-10.7) |
| | $D_{OH}$ | 17.5(11.0) | 18.8(12.0) | -10.3(-16.4) |
| **$HIO_2$···$H_2O$** | **$AD_OW_{IO}$** | **44.4(32.2)** | **47.6(35.0)** | **7.7(-3.9)** |
| | $D_OE_{IO}$ | 34.4(26.8) | 36.1(28.7) | -0.7(-8.7) |
| | $D_OW_{IO}$ | 29.6(21.4) | 31.0(22.3) | -1.9(-8.4) |
| | $D_{OH}E_{IO}$ | 28.8(17.5) | 29.8(18.2) | -5.4(-15.9) |
| **$HIO_3$···$H_2O$** | **$AD_OW_{IO}$** | **43.0(36.1)** | **47.3(40.5)** | **4.3(-3.3)** |
| | $D_O{}^2E_{IO}$ | 37.6(31.0) | 39.2(32.5) | 3.7(-3.5) |
| | $D_OD_{OH}E_{IO}$ | 33.7(23.1) | 36.2(25.4) | -4.4(-14.9) |
| **$HIO_4$···$H_2O$** | **$AD_OW_{IO}$** | **46.1(39.8)** | **49.6(43.3)** | **11.4(3.0)** |
| | $D_{OH}{}^2E_{IO}$ | 30.5(24.1) | 32.7(26.4) | -7.0(-13.6) |

**Table S3.** MP2(B3LYP) binding energies ($-\Delta E_e$), zero-point energy (ZPE) corrected binding energies ($-\Delta E_0$), binding enthalpies ($-\Delta H_r$) and free binding energies ($-\Delta G_r$) [in kJ/mol] at room temperature and 1 bar for various conformers of $HBrO_{n=0-4}$···water complexes where the aVDZ basis set was used except for bromine for which the CRENBL ECP basis set was employed.

| acid···water | Conformer | $-\Delta E_e$ | $-\Delta E_0$ | $-\Delta H_r$ | $-\Delta G_r$ |
|---|---|---|---|---|---|
| **HBr···$H_2O$** | **$A_H$** | **23.6(18.2)** | **15.7(11.3)** | **18.4(13.6)** | **-8.9(-12.8)** |
| | $W_{BrO}$ | 5.8(3.5) | 2.6(-0.3) | 1.7(-0.6) | -11.9(-17.9) |
| **HBrO···$H_2O$** | **A** | **30.6(27.0)** | **22.0(18.7)** | **23.3(20.0)** | **-6.2(-9.2)** |
| | $E_{BrO}$ | 21.6(18.0) | 16.7(13.2) | 16.1(13.1) | -12.0(-16.4) |
| | $D_{OH}$ | 24.2(-) | 16.1(-) | 17.6(-) | -12.3(-) |
| **$HBrO_2$···$H_2O$** | **$AD_OW_{BrO}$** | **56.0(44.6)** | **45.0(34.2)** | **48.6(37.6)** | **7.8(-2.6)** |
| | $D_O E_{BrO}$ | 33.8(24.5) | 27.7(17.8) | 27.9(18.5) | -1.3(-14.3) |
| | $D_O W_{BrO}$ | 34.9(25.4) | 26.7(18.2) | 28.1(19.0) | -4.5(-10.9) |
| | $D_{OH} E_{BrO}$ | 31.6(20.1) | 25.4(13.9) | 25.9(14.2) | -7.2(-17.7) |
| **$HBrO_3$···$H_2O$** | **$AD_OW_{BrO}$** | **49.4(43.9)** | **38.0(32.5)** | **41.8(36.7)** | **1.1(-6.5)** |
| | $D_O^2 E_{BrO}$ | 35.4(26.8) | 29.0(20.2) | 29.5(20.8) | -3.2(-12.0) |
| | $D_O D_{OH} E_{BrO}$ | 36.7(24.8) | 29.5(17.7) | 30.5(18.6) | -4.3(-16.0) |
| **$HBrO_4$···$H_2O$** | **$AD_OW_{BrO}$** | **55.3(47.9)** | **44.4(37.7)** | **47.9(41.2)** | **6.8(-1.9)** |
| | $AD_OW_{BrO}$ | 53.3(47.9) | 43.2(37.7) | 46.4(41.2) | 6.9(-0.5) |

**Table S4.** MP2/aVDZ scaled harmonic ($\nu^S$) (scaled by 0.957) and anharmonic vibrational frequencies ($\nu^{anh}$) of -OH stretching modes [$cm^{-1}$] for the most stable conformers. The subscripts denote IR intensities [10 km/mol]. The underlined values correspond to –OH vibrations of OH group which is not involved in hydrogen bond formation.

| acid···water | Structure | $\nu^s$ | $\nu^{anh}$ |
|---|---|---|---|
| $HBO_2$···$H_2O$ | A | $3298_{130}$ $\underline{3631_2}$ $\underline{3752_{11}}$ | $3275_{130}$ $\underline{3618_2}$ $\underline{3725_{11}}$ |
| $H_3BO_3$···$H_2O$ | $AD_{OH}$ | $3464_{40}$ $3557_{22}$ $\underline{3687_7}$ $\underline{3691_{16}}$ $3729_{12}$ | $3441_{40}$ $3535_{22}$ $\underline{3666_7}$ $\underline{3671_{16}}$ $3708_{12}$ |
| HCN···$H_2O$ | $A_H$ | $\underline{3212_{36}}$ $\underline{3764_9}$ | $\underline{3200_{36}}$ $\underline{3725_9}$ |
| $HNO_2$···$H_2O$ | $A(D_O)$ | $3171_{61}$ $3614_1$ $3744_{10}$ | $3157_{61}$ $3601_1$ $3724_{10}$ |
| $HNO_2$···$H_2O$ | A | $3324_{82}$ $\underline{3626_2}$ $\underline{3749_{10}}$ | $3318_{82}$ $\underline{3611_2}$ $\underline{3728_{10}}$ |
| $HNO_3$···$H_2O$ | $AD_O$ | $3143_{100}$ $3608_2$ $3738_{12}$ | $3067_{100}$ $3589_2$ $3713_{12}$ |
| HF···$H_2O$ | $A_H$ | $\underline{3635_1}$ $\underline{3756_{11}}$ | $\underline{3617_1}$ $\underline{3734_{11}}$ |
| $P(OH)_3$···$H_2O$ | $AD_OW_{PO}$ | $3261_{54}$ $3544_{14}$ $\underline{3629_9}$ $\underline{3646_{10}}$ $3706_{10}$ | $3209_{54}$ $3527_{14}$ $\underline{3609_9}$ $\underline{3631_{10}}$ $3680_{10}$ |
| $H_3PO_3$···$H_2O$ | $AD_{OH}W_{PO}$ | $3191_{69}$ $3428_{42}$ $\underline{3629_{12}}$ $3716_{11}$ | $3106_{69}$ $3380_{42}$ $\underline{3607_{12}}$ $3693_{11}$ |
| $H_3PO_4$···$H_2O$ | $AD_OW_{PO}$ | $3187_{76}$ $3445_{37}$ $\underline{3638_{12}}$ $\underline{3641_{11}}$ $3715_{11}$ | $3103_{76}$ $3398_{37}$ $\underline{3617_{12}}$ $\underline{3621_{11}}$ $3692_{11}$ |
| $H_2S$···$H_2O$ | $D_S$ | $3582_{15}$ $3738_{16}$ | $3576_{15}$ $3720_{16}$ |
| $H_2S$···$H_2O$ | $A_H$ | $\underline{3634_1}$ $\underline{3761_8}$ | $\underline{3615_1}$ $\underline{3739_8}$ |
| $(HO)_2SO$···$H_2O$ | $A^2D_OW_{SO}$ | $3416_0$ $3426_{24}$ $3491_{27}$ $3722_{11}$ | $3360_0$ $3364_{24}$ $3465_{27}$ $3691_{11}$ |
| $(HO)_2SO$···$H_2O$ | $AD_OW_{SO}$ | $3071_{77}$ $3499_{17}$ $\underline{3561_8}$ $3708_{10}$ | $2978_{77}$ $3467_{17}$ $\underline{3537_8}$ $3681_{10}$ |
| $H_2SO_3$···$H_2O$ | $A^2D_OW_{SO}$ | $3037_{116}$ $3550_{10}$ $3718_{14}$ | $2945_{116}$ $3523_{10}$ $3692_{14}$ |
| $H_2SO_4$···$H_2O$ | $AD_OW_{SO}$ | $3038_{117}$ $3562_8$ $\underline{3572_{12}}$ $3720_{14}$ | $2946_{117}$ $3541_8$ $\underline{3544_{12}}$ $3694_{14}$ |
| $H_2Se$···$H_2O$ | $D_{Se}$ | $3579_{18}$ $3736_{15}$ | $3570_{18}$ $3718_{15}$ |
| HCl···$H_2O$ | $A_H$ | $3624_2$ $3745_9$ | $3608_2$ $3728_9$ |
| HClO···$H_2O$ | A | $3340_{71}$ $\underline{3627_2}$ $\underline{3750_{10}}$ | $3334_{71}$ $\underline{3615_2}$ $\underline{3728_{10}}$ |
| $HClO_2$···$H_2O$ | $AD_OE_{ClO}$ | $3264_{45}$ $3477_{25}$ $3723_9$ | $3205_{45}$ $3451_{25}$ $3702_9$ |
| $HClO_3$···$H_2O$ | $AD_OW_{ClO}$ | $3105_{71}$ $3580_4$ $3716_{10}$ | $3063_{71}$ $3566_4$ $3692_{10}$ |
| $HClO_4$···$H_2O$ | $AD_O{}^2W_{ClO}$ | $3034_{106}$ $3604_2$ $3726_{11}$ | $2965_{106}$ $3586_2$ $3697_{11}$ |
| $HClO_4$···$H_2O$ | $AD_OW_{ClO}$ | $3053_{110}$ $3606_2$ $3735_{12}$ | $3008_{110}$ $3587_2$ $3711_{12}$ |
| HBr···$H_2O$ | $A_H$ | $3626_2$ $3751_9$ | $3612_2$ $3734_9$ |
| HBrO···$H_2O$ | A | $3347_{72}$ $\underline{3627_2}$ $\underline{3750_9}$ | $3333_{72}$ $\underline{3621_2}$ $\underline{3731_9}$ |
| $HBrO_2$···$H_2O$ | $AD_OW_{BrO}$ | $3275_{30}$ $3437_{27}$ $3723_{10}$ | $3205_{30}$ $3395_{27}$ $3702_{10}$ |
| $HBrO_3$···$H_2O$ | $AD_OW_{BrO}$ | $3047_{80}$ $3532_{10}$ $3709_{11}$ | $2967_{80}$ $3503_{10}$ $3685_{11}$ |
| $HBrO_4$···$H_2O$ | $AD_OW_{BrO}$ | $2995_{108}$ $3590_3$ $3720_{12}$ | $2881_{108}$ $3568_3$ $3692_{12}$ |
| $HBrO_4$···$H_2O$ | $AD_OW_{BrO}$ | $2960_{130}$ $3589_3$ $3728_{14}$ | $2887_{130}$ $3568_3$ $3701_{14}$ |
| HI···$H_2O$ | $A_H$ | $3627_2$ $3754_8$ | $3613_2$ $3736_8$ |
| HI···$H_2O$ | $D_I$ | $3603_{13}$ $3742_{17}$ | $3583_{13}$ $3717_{17}$ |
| HIO···$H_2O$ | $E_{IO}$ | $\underline{3611_9}$ $\underline{3622_3}$ $\underline{3748_{10}}$ | $\underline{3592_9}$ $\underline{3605_3}$ $\underline{3726_{10}}$ |
| HIO···$H_2O$ | A | $3406_{62}$ $\underline{3629_1}$ $\underline{3753_9}$ | $3401_{62}$ $\underline{3609_1}$ $\underline{3725_9}$ |
| $HIO_2$···$H_2O$ | $AD_OW_{IO}$ | $3311_2$ $3365_{62}$ $3719_9$ | $3237_2$ $3293_{62}$ $3695_9$ |
| $HIO_3$···$H_2O$ | $AD_OW_{IO}$ | $3060_{75}$ $3445_{26}$ $3705_{11}$ | $2942_{75}$ $3395_{26}$ $3679_{11}$ |
| $HIO_4$···$H_2O$ | $AD_OW_{IO}$ | $2906_{140}$ $3551_8$ $3716_{15}$ | $2730_{140}$ $3516_8$ $3689_{15}$ |

**Table S5.** MP2/aVDZ scaled harmonic ($\nu^S$) (scaled by 0.957) vibrational frequencies of -OH stretching modes [$cm^{-1}$] for less stable conformers. The subscripts denote IR intensities [10 km/mol]. The underlined values correspond to –OH vibrations of OH group which is not involved in hydrogen bond formation.

| acid···water | conformer | $\nu^s$ |
|---|---|---|
| $HCN\cdots H_2O$ | $D_N$ | $3594_{19}$ $3743_{14}$ |
| $HNO_2\cdots H_2O$ | A | $3324_{82}$ $\underline{3626}_2$ $\underline{3749}_{10}$ |
| | $D_{OH}$ | $\underline{3566}_9$ $3595_{12}$ $3744_{14}$ |
| | $D_O$ | $\underline{3410}_4$ $3621_9$ $3753_{16}$ |
| $HNO_3\cdots H_2O$ | $D_{OH}W_{NO}$ | $\underline{3546}_9$ $3631_1$ $3758_7$ |
| | $D_O^2$ | $\underline{3540}_{10}$ $3629_5$ $3747_8$ |
| | $D_O$ | $\underline{3538}_{11}$ $3780_9$ $3919_{16}$ |
| $P(OH)_3\cdots H_2O$ | A | $3412_{82}$ $\underline{3628}_1$ $\underline{3639}_9$ $\underline{3642}_9$ $\underline{3752}_9$ |
| $H_3PO_3\cdots H_2O$ | $AD_{OH}W_{PO}$ | $3320_{72}$ $3590_6$ $\underline{3622}_{12}$ $3738_{13}$ |
| | $D_{OH}^2W_{PO}$ | $\underline{3618}_{14}$ $\underline{3619}_{12}$ $3624_0$ $3741_7$ |
| | $D_{OH}W_{PO}$ | $3610_6$ $3623_{13}$ $3625_{10}$ $3750_{12}$ |
| $H_3PO_4\cdots H_2O$ | $AD_{OH}W_{PO}$ | $3257_{83}$ $3591_5$ $\underline{3631}_{12}$ $\underline{3639}_{12}$ $3727_{12}$ |
| $H_2S\cdots H_2O$ | $A_H$ | $\underline{3634}_1$ $\underline{3761}_8$ |
| $(HO)_2SO\cdots H_2O$ | $AD_OW_{SO}$ | $3071_{77}$ $3499_{17}$ $\underline{3561}_8$ $3708_{10}$ |
| | $AD_{OH}W_{SO}$ | $3308_{56}$ $\underline{3514}_8$ $3579_6$ $3735_{13}$ |
| | $D_{OH}^2W_{SO}$ | $\underline{3518}_6$ $\underline{3520}_{10}$ $3624_1$ $3742_6$ |
| | $D_{OH}W_{SO}$ | $\underline{3516}_6$ $\underline{3518}_{10}$ $3615_5$ $3751_{12}$ |
| $H_2SO_3\cdots H_2O$ | $AD_O^2W_{SO}$ | $\underline{3575}_{12}$ $3617_1$ $3737_8$ |
| | $A_H$ | $\underline{3575}_{11}$ $\underline{3627}_2$ $\underline{3752}_9$ |
| $H_2SO_4\cdots H_2O$ | $A^2D_OW_{SO}$ | $3447_1$ $3469_{45}$ $3573_6$ $3731_{13}$ |
| | $D_O$ | $\underline{3571}_{10}$ $\underline{3575}_{16}$ $3610_{11}$ $3747_{16}$ |
| $H_2Se\cdots H_2O$ | $A_H$ | $3633_1$ $3761_8$ |
| $HClO\cdots H_2O$ | $E_{ClO}$ | $\underline{3589}_7$ $\underline{3628}_1$ $\underline{3755}_8$ |
| $HClO_2\cdots H_2O$ | $D_OW_{ClO}$ | $\underline{3528}_{13}$ $3539_{20}$ $3737_{12}$ |
| | $D_{OH}E_{ClO}$ | $\underline{3525}_6$ $3598_4$ $3746_{11}$ |
| $HClO_3\cdots H_2O$ | $D_{OH}E_{ClO}$ | $\underline{3505}_6$ $3554_{11}$ $3735_{11}$ |
| | $D_O^2E_{ClO}$ | $\underline{3494}_6$ $3626_2$ $3751_8$ |
| | $D_{OH}$ | $\underline{3495}_7$ $3571_{21}$ $3738_{14}$ |
| $HClO_4\cdots H_2O$ | $AD_OW_{ClO}$ | $3053_{110}$ $3606_2$ $3735_{12}$ |
| | $D_O$ | $\underline{3504}_{11}$ $3636_3$ $3761_{15}$ |
| $HBr\cdots H_2O$ | $W_{BrO}$ | $\underline{3636}_1$ $\underline{3764}_7$ |
| $HBrO\cdots H_2O$ | $E_{BrO}$ | $\underline{3591}_8$ $\underline{3624}_2$ $\underline{3750}_8$ |
| | $D_{OH}$ | $\underline{3559}_8$ $3580_{18}$ $3742_{14}$ |
| $HBrO_2\cdots H_2O$ | $D_OE_{BrO}$ | $\underline{3549}_9$ $3589_2$ $3735_{10}$ |
| | $D_OW_{BrO}$ | $3497_{36}$ $\underline{3540}_8$ $3733_{11}$ |
| | $D_{OH}E_{BrO}$ | $\underline{3537}_8$ $3596_2$ $3742_{11}$ |
| $HBrO_3\cdots H_2O$ | $D_O^2E_{BrO}$ | $\underline{3497}_9$ $3609_2$ $3730_8$ |
| | $D_OD_{OH}E_{BrO}$ | $\underline{3494}_8$ $3610_1$ $3730_8$ |
| $HBrO_4\cdots H_2O$ | $AD_OW_{BrO}$ | $2960_{130}$ $3589_3$ $3728_{14}$ |
| $HI\cdots H_2O$ | $D_I$ | $3603_{13}$ $3742_{17}$ |
| | $W_{IO}$ | $\underline{3637}_1$ $\underline{3764}_8$ |
| $HIO\cdots H_2O$ | A | $3406_{62}$ $\underline{3629}_1$ $\underline{3753}_9$ |
| | $D_{OH}$ | $3532_{30}$ $\underline{3583}_{11}$ $3733_{13}$ |
| $HIO_2\cdots H_2O$ | $D_OE_{IO}$ | $3490_8$ $\underline{3579}_{10}$ $3706_{11}$ |
| | $D_OW_{IO}$ | $3402_{57}$ $\underline{3571}_{10}$ $3728_{10}$ |
| | $D_{OH}E_{IO}$ | $3562_7$ $\underline{3566}_7$ $3731_{12}$ |
| $HIO_3\cdots H_2O$ | $D_O^2E_{IO}$ | $\underline{3539}_{11}$ $3572_3$ $3690_9$ |
| | $D_OD_{OH}E_{IO}$ | $\underline{3516}_{10}$ $3584_2$ $3703_8$ |
| $HIO_4\cdots H_2O$ | $D_{OH}^2E_{IO}$ | $\underline{3533}_{14}$ $3573_4$ $3697_{10}$ |